

Alanine, 2-methyl-
62-57-7 | DTXSID0058772

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 9.33 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,4-Dioxane</div> <div>Measured: 17.0</div> <div>Predicted: 13.2</div>	<div>Image not found</div> <div>2,2'-Bioxirane</div> <div>Measured: 2.51</div> <div>Predicted: 4.97</div>	<div>Image not found</div> <div>1,2-Propylene glycol</div> <div>Measured: 2.29</div> <div>Predicted: 4.24</div>
<div>Image not found</div> <div>Acrylamide</div> <div>Measured: 50.1</div> <div>Predicted: 16.7</div>	<div>Image not found</div> <div>1,2-Diethylhydrazine</div> <div>Measured: 15.1</div> <div>Predicted: 14.1</div>	